

4-Hydroxybenzoic acid
99-96-7 | DTXSID3026647

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 242 °C

Global applicability domain: Inside

Local applicability domain index: 2.59e-01

Confidence level: 3.39e-01

Nearest Neighbors from the Training Set

Image not found

2-Hydroxyphenylacetic acid

Measured: 240

Predicted: 261

Image not found

2-Chlorobenzoic acid

Measured: 287

Predicted: 273

Image not found

Chloral hydrate

Measured: 98.0

Predicted: 123

Image not found

Benzoic acid, 4-methoxy-

Measured: 277

Predicted: 279